Experimental Group on Electron Spectroscopy(Annual Report)

Experimental Group on Electron Spectroscopy

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Research Activities

(I) PHOTOELECTRON SPECTROSCOPY

(A) Angle-Resolved Ultraviolet Photoelectron Spectroscopy (ARUPS) and the Band Structures

1) Black Phosphorus

The ARUPS measurements on the black P single crystal were successfully performed by the HeI, NeI and ArI resonance lines with high augular and energy resolutions of 1.5° or less and 0.1 eV, respectively. The experimentally derived band structure has been compared with the self-consistent pseudopotential calculations. The experimental result corresponds well to the calculations as a whole, though of course not in fine details. Typically the 3p derived band width is rather narrow in experiments than calculations. It has been found that some special points and bands can be assigned unambiguously and are very useful to improve the numerical parameters to be employed in the band calculations.

In conjunction with the ARUPS measurements, we are carrying out the experiments on the Kβ x-ray fluorescence spectra and also on the K absorption spectra of the black P single erystal in order to get imformations about the density of states of P_x, P_y and P_z components.

2) Grey Arsenic

The ARUPS spectra of grey As were obtained already. However, an analysis of the results is still under groping in the dark, because the energy dispersions along the normal direction to the surface are rather large for almost all bands despite its easy cleaving nature along the surface.

3) P-As Alloys with A-11 Crystal Structure

The ARUPS measurement is intended in near future for the purpose of comparisons with the results for P and As.

(B) XPS Studies on the 4f Levels in Rare Earth Metal Compounds

The XPS measurements of the 4f levels in YbB_6, YbB_{12}, TmB_{12} and LuB_{12} were intended in collaboration with the experimental group on magnetism. Our main concern in these measurements is to know whether the valence mixing does exist or not. In the preliminary study on YbB_{12}, we found weak but clear $4f^{14}$ multiplet structures at the vicinity of Fermi energy and the strong $4f^{13}$ multiplets shifted about 7.0 eV toward low energy side from the $4f^{14}$ spectra. In YbB_6, only the $4f^{14}$ multiplets were observed at $E_B \approx 1$ eV as expected.

In the course of study it has become evident that the four-components structure in Yb metal 4f levels is due to surface effect of intrinsic nature.

(C) Photoemission Studies on Amorphous Materials

1) Highly Disordered Amorphous Se

XPS has been applied to a highly disordered amorphous Se deposited onto a cooled (150K) substrate. The spectral changes have been observed in the 4p bonding and 4s states upon annealing of the film. The thermal growth of the upper 4p bonding band is in good agreement with previous UPS measurements. The 4s band of the highly disordered film shows a round and narrow feature and transforms into a rectangular shape upon the annealing. The change of the 4s band is explained by a thermally induced increase of the cluster size in the cluster-junction model proposed in the previous UPS study.

2) Crystallization of Amorphous GeTe Film

The UPS and XPS spectra of amorphous GeTe film exhibit a drastic change upon annealing and/or the crystallization of the film. It was found that an amorphous GeTe film deposited onto a room temperature substrate has a 4-2 coordinated local structure, while a highly disordered amorphous GeTe film evaporated onto a cooled (77K) substrate is largely 3-3 coordinated, and relaxes into the 4-2 structure upon annealing within amorphous phase.

3) Local Structure of Amorphous GeSe Film

XPS and UPS spectra have been measured for an amorphous GeSe film deposited onto a cooled substrate before and after annealing of the film. The spectra show a remarkable change in the 4p and the Ge4s region. A comparison of the results with the recently presented electronic structure calculations reveals that an amorphous GeSe film deposited onto a cooled

substrate has a 3-3 coordination character and relaxes into a chemically ordered 4-2 coordinated structure upon annealing.

(II) STUDY ON SURFACE ELECTRONIC STRUCTURES BY MEANS OF ARUPS

(A) Temperature Dependence of Surface Electronic Structure of Si(111)

temperature dependence of ARUPS has been observed for Si(111) surfaces starting with a thermally quenched "1x1" surface and ending with a high temperature "1x1" surface. It has been found that the surface state at 0.8 eV below the Fermi level exhibits degradation with the increase in temperature, which explains the diffrence of surface electronic structures between a quenched "1x1" surface and a high temperature "1x1" surface. Electron correlation effect in a dangling-bond derived surface state is postulated as a cause for the phenomena.

(B) Electronic Structures of Ge(111)7x7-Sn and Ge(111)2x8 Surfaces

ARUPS have shown that the surface electronic structure of a Ge(111) 7x7-Sn surface is essentially the same as that of a Si(111)7x7 surface. Metallic surface states of a Ge(111)7x7-Sn surface reveal a slight dispersion of 2x2 periodicity. The so-called dangling-bond and the back-bond surface states for a Ge(111)7x7-Sn surface lie at essentially the same binding energies as those for a Ge(111)2x8 surface.

(C) Electronic Structure of Ag/Si(111) Submonolayer Interface

ARUPS spectra have been measured for well-defined Ag/Si(111) submonolayer interface of (1) Si($\sqrt{3}$x$\sqrt{3}$)R30°-Ag, (2) "Si(111)6x1 -Ag" and (3)Ag/Si(111) as deposited at room temperature. Non-dispersive and very narrow (FWHM$\sim$0.4$\sim$0.5 eV)Ag 4d derived peaks are found at 5.6 and 6.5 eV below the Fermi level for surface (1) and at 5.3 and 6.0 eV for surface (2). Dispersions of sp "binding" states in the energy range between E_F and Ag 4d states have been precisely determined for surface (1). Electronic structures similar to those of the Ag(111) surface, including the surface state near E_F, have been observed for surface (3).

(III) STUDY ON SURFACE ATOMIC GEOMETRY BY MEANS OF AUGER ELECTRON DIFFRACTION AND X-RAY PHOTOELECTRON DIFFRACTION

(A) Ag(110)Surface

$AgM_4N_{4,5}N_{4,5}$ Auger electron diffraction and Ag 3d X-ray photoelectron diffraction from Ag(110) surface have been measured and interpreted kinematically. There is very good agreement between the experiment and the interpretation showing the applicability of the kinematical interpretation.

(B) Si(111)($\sqrt{3}$x$\sqrt{3}$)R30°-Ag Surface

Final state diffraction of Ag 3d x-ray photoelectron from Si(111) ($\sqrt{3}$x$\sqrt{3}$)R30°-Ag surface has been measured. From a kinematical analysis

of the diffraction patterns, it is found that a buried honeycomb framework of Ag atoms is formed on the surface with lateral displacement of the first Si layer.

(C) Ge(111)2x8 Surface

Ge $L_3M_{4,5}M_{4,5}$ Auger electron diffraction from the Ge(111) 2x8 surface has been measured and analyzed kinematically. Very good agreement between the experiment and the calculation for the truncated Ge(111)1x1 surface has been reached which shows not only the validity of the kinematical interpretation but also the insensitivity of the Auger electron diffraction to the 2x8 reconstruction.

(D) Ge(111)7x7-Sn Surface

X-ray photoelectron diffraction of Sn3d core levels for Ge(111)7x7-Sn surface has been measured and analyzed. Based on the finding of Ichikawa and Ino that the Ge(111)7x7-Sn and Si(111)7x7 surfaces have essentially the same structures, the analysis is aimed to explain the structure of the 12 maxima found in the recent scanning tunneling microscopy for Si(111)7x7 surface. A "tri-pedal" model is proposed in which a compressed tetrahedron of four atoms stands on three first-layer atoms.

(E) Ge(111)($\sqrt{3}$x$\sqrt{3}$)R30°-Sn Surface

Azimuthal angle dependence of Sn 3d X-ray photoelectron diffraction from Ge(111)($\sqrt{3}$x$\sqrt{3}$)R30°-Sn surface has been measured and analyzed kinematically. It has been found that triplets of Sn atoms, the side of the triplet being 3.1±0.1Å, are formed on the substrate surface although the bonding sites of the triplets to the substrate are yet to be determined.

Doctor Thesis

(D1) A Study on the Edge Anomaly in the $L_{2,3}$ Emission Bands of Al-Mg Alloys, C. Y. Park

Master Thesis

(M1) Study on Surface Atomic Structures of Sn/Ge(111) Systems by means of the Auger electron diffraction and the X-ray photoelectron, Hiroshi Sakurai

Publications

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10) Band Structure of Black Phosphous Studied by Angle-Resolved Ultraviolet Photoemission Spectroscopy, Solid State Communications 45(1983)945
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